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Classification and Dose-Response Characterization of Environmental Chemicals based on Structured Toxicity Information from ToxRefDB

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Thirty years and over a billion of today's dollars worth of pesticide registration toxicity studies, historically stored as hardcopy and scanned documents, have been digitized into highly standardized and structured toxicity data, within the U.S. Environmental Protection Agency's (EPA) Toxicity Reference Database (ToxRefDB). The source toxicity data in ToxRefDB covers multiple study types, including subchronic, developmental, reproductive, chronic, and cancer studies, resulting in a diverse set of endpoints and toxicities. Novel approaches to chemical classification are performed as a model application of ToxRefDB and as an essential need for highly detailed chemical classifications within the EPA's ToxCast™ research program. In order to develop predictive models and biological signatures utilizing high-throughput screening (HTS) and *in vitro* genomic data, endpoints and toxicities must first be identified and globally characterized for ToxCast Phase I chemicals. Secondarily, dose-response characterization within and across toxicity endpoints provide insight into key precursor toxicity events and overall endpoint relevance. Toxicity-based chemical classification and dose-response characterization utilizing ToxRefDB prioritized toxicity endpoints and differentiated toxicity outcomes across a large chemical set. *This work was reviewed by EPA and approved for publication but does not necessarily reflect official Agency policy.*